

# An Interactive Complex Hermitian-Lanczos Eigensolver

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## Abstract

This report describes a Lanczos algorithm based code intended for the solution of eigenproblems involving complex Hermitian matrices. The code works in an interactive way with the user, who has access to intermediate computed results (the convergence history) and can thus define specialized external control instructions. In addition, the Hermitian matrix is not required internally in the package for the generation of the Lanczos vectors basis: each time a matrix-vector computation has to be performed the control is returned to the user. The fundamentals of the technique are first reviewed, including a comparison between the reduced problem obtained by the adopted formulation and a block one, and the strategy employed to preserve the orthogonality among the vectors of the basis generated. Then, some applications and conclusions are presented. Finally, a user's guide for the code, called HLZPACK (an acronym for Hermitian Lanczos Package), is given in the Appendix.

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# 1 Introduction

A large number of applications require the determination of non-trivial solutions for a problem of the type

$$Ax = \lambda x \quad (1)$$

where  $A$  is an  $n \times n$  matrix,  $x$  is a  $n$ -vector and  $\lambda$  is a scalar. When  $A$  is sparse and a few pairs of *eigenvalues*  $\lambda$  and *eigenvectors*  $x$  are sought, Krylov subspace based methods have been shown to be very suited for their computation. For a given non-null vector  $q$ , a Krylov subspace is defined as [8, 14]

$$\mathcal{K}(A, q, j) = \text{span}(q, Aq, \dots A^{j-1}q). \quad (2)$$

The vectors of such a subspace are similar to those generated by the power method [8, 14] and as  $j$  increases convergence is achieved for the eigenvector with predominant components in  $q$ . However, a more general approach consists in generating a basis for  $\mathcal{K}(A, q, j)$ , in order to achieve convergence for more solutions. This is the governing idea of the Lanczos [11, 14] and Arnoldi [1, 8] methods, which start with a vector  $q_1$  and at each step  $j$  add a new vector,  $q_j$ , to the basis. The projection of the original problem (1) onto the basis leads to a small problem, either involving a tridiagonal (one-vector or basic Lanczos) or an upper Hessenberg matrix (one-vector or basic Arnoldi), which are easier to solve. The solutions required for the large eigenproblem are then recovered through a Rayleigh-Ritz procedure. In a block Krylov based strategy (block Lanczos or Arnoldi)  $q_1$  is replaced by a full rank  $n \times p$  matrix, leading to a block tridiagonal or block Hessenberg matrix and better convergence properties in the case of clustered or multiple eigenvalues [8, 9, 14, 16].

Let us consider now a matrix defined as  $A = P + iZ$ , where  $P$  is real and symmetric,  $Z$  is real ( $\neq 0$ ) and *skew* symmetric<sup>†</sup>, and  $i$  denotes the complex unit ( $\sqrt{-1}$ ). For this type of matrix, all associated eigenvalues are real while the eigenvectors are complex [18]. In addition, if  $(\lambda, x)$  corresponds to an eigenpair with  $x^*x = 1$ <sup>‡</sup>, so does  $(\lambda, \xi x)$  providing  $\xi$  is a complex number satisfying  $\bar{\xi}\xi = 1$ <sup>¶</sup>. When  $P = 0$ ,  $A$  is said to be *pure imaginary Hermitian*, and its eigensolutions appear as pairs  $(\lambda, x)$  and  $(-\lambda, \bar{x})$ , with one  $\lambda = 0$  for an odd value of  $n$ . Gupta and Lawson [10, 12], for instance, developed a block Lanczos code for such a kind of problem, intended for the analysis of spinning structures like helicopters and turbines. They showed that  $A$  can be projected onto a real basis without damaging the convergence properties. The complex arithmetic is “forced” to be only in the reduced problem. When  $P \neq 0$ , the resulting matrix  $A$  is said to be *general Hermitian* ( $A = A^*$ ), which will be referred to as  $\mathcal{H}$  henceforth. Such matrices appear, for example, in electromagnetism applications and in the spectral analysis of nonsymmetric matrices (within a singular value decomposition strategy). Then, if the one-vector Lanczos method is employed, the basis generated is complex but the reduced problem corresponds to a real symmetric tridiagonal matrix. This contrasts with the block Lanczos method, which leads to a block tridiagonal complex Hermitian matrix. It should be noted that Cullum and Willoughby [5] have already developed a Fortran code using the real formulation for the reduced problem. Their code, however, uses some constructions and complex functions that are not standard. In addition, it somewhat restricts the user to specific data structures.

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<sup>†</sup>  $Z = -Z^T$ .

<sup>‡</sup> the  $*$  denotes the conjugate transpose, i.e.  $x^* = \bar{x}^T$ .

<sup>¶</sup>  $\bar{\xi}\xi = 1$  defines a circle of unitary radius.

Therefore, the purpose of this work is to describe a “friendly” tool for the determination of some of the extreme solutions of eigenproblems associated with complex Hermitian matrices. A single-vector Lanczos approach is used, which has the characteristics mentioned above. The main goal is to give to the user the possibility of using the code as a function, in an interactive fashion (reverse communication strategy). In terms of user interface, the features of the proposed “Hermitian-Lanczos” code are thus the following:

- the user has access to intermediate results and to the convergence history, which allows the definition of specific control instructions outside the package.
- the Hermitian matrix is not required internally in the code: until convergence for the required solutions is reached, each time a computation involving  $\mathcal{H}$  and a given vector  $q_j$  has to be performed, the control is returned to the user (and such a computation can be then specialized for particular applications).

In the following sections, the fundamentals of the Hermitian-Lanczos code are first described. We include a discussion about the reduced problem used here and the one obtained by a block formulation. Next we show the strategy adopted to maintain the basis of vectors with a proper level of orthogonality. Then, four examples are given in order to illustrate the applicability of the code: a small matrix and the convergence pattern using a direct and an inverted operator ( $\mathcal{H}$  and  $\mathcal{H}^{-1}$ ), the evaluation of a spectral portrait of a nonsymmetric matrix (with a singular value decomposition scheme), and the determination of some singular values of a complex nonsymmetric matrix using an augmented matrix strategy. Finally, some conclusions are presented, as well as a user’s guide for the package.

## 2 Fundamentals

The Gram-Schmidt orthonormalization process could be applied to all vectors of the Krylov subspace, in the natural order  $q, Aq, A^2q, \dots$ , so as to construct a basis for it. However, one can show that for the orthonormalization of the  $k$ -th vector it suffices to take into account only the two previous orthonormalized vectors. Moreover, instead of generating the Krylov subspace, the basis can be built vector by vector, which is one of the characteristics of the Lanczos method [14]. Considering the eigenproblem

$$\mathcal{H}x = \lambda x, \quad (3)$$

the basis generation process starting from a vector  $q_1$  is summarized in Table 1. In that table, the  $n$ -vectors  $q_j$  and  $r_j$  are complex while the scalars  $\alpha_j$  and  $\beta_j$  are real (their nature will be discussed in the next section).

After  $j$  steps the vectors generated can be arranged as

$$Q_j = \begin{bmatrix} q_1 & q_2 & \dots & q_j \end{bmatrix} \quad (4)$$

satisfying

$$Q_j^* Q_j = I \quad (5)$$

Table 1: The Lanczos basis generation process.

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set $q_0 = 0$ and $\beta_1 = 0$
set $q_1 \neq 0$ so that $q_1^* q_1 = 1$
for $j=1,2,\dots$
a) $r_j \leftarrow \mathcal{H}q_j$
b) $r_j \leftarrow r_j - q_{j-1}\beta_j$
c) $\alpha_j \leftarrow q_j^* r_j$
d) $r_j \leftarrow r_j - q_j \alpha_j$
e) $\beta_{j+1} \leftarrow \sqrt{r_j^* r_j}$
f) $q_{j+1} \leftarrow \frac{1}{\beta_{j+1}} r_j$

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so that

$$\mathcal{Q}_j^* \mathcal{H} \mathcal{Q}_j = T_j \quad (6)$$

where

$$T_j = \begin{bmatrix} \alpha_1 & \beta_2 & & & \\ \beta_2 & \alpha_2 & \beta_3 & & \\ & \beta_3 & \alpha_3 & \ddots & \\ & & \ddots & \ddots & \beta_j \\ & & & \beta_j & \alpha_j \end{bmatrix}. \quad (7)$$

Therefore, the operations listed in Table 1 lead to a partial tridiagonalization of  $\mathcal{H}$ . Defining  $\mathcal{Q}_n$  as the basis that completely tridiagonalizes  $\mathcal{H}$ , i.e.,  $j = n$  in relation (6), the truncated scheme is depicted in Figure 1. In terms of the Rayleigh-Ritz approximation, the projection of the eigenproblem (3) onto the *trial* basis  $\mathcal{Q}_j$  is the symmetric tridiagonal matrix  $T_j$ , with an approximate solution  $(\hat{\lambda}, \hat{x})$  given by

$$\hat{\lambda} = \theta_l \quad (8)$$

and

$$\hat{x} = \mathcal{Q}_j s_l \quad (9)$$

with  $(\theta_l, s_l)$ ,  $1 \leq l \leq j$ , satisfying the reduced eigenproblem

$$T_j s_l = s_l \theta_l, \quad (10)$$

which can be solved by means of Givens rotations or a bisection method [18], for example, and  $\hat{x}^* \hat{x} = 1$  providing  $s_l^T s_l = 1$ . Convergence is usually achieved for  $j \ll n$  and the accuracy of  $(\hat{\lambda}, \hat{x})$  can be estimated *a priori*, through the residual (see Figure 1)

$$\|\mathcal{H}\hat{x} - \hat{\lambda}\hat{x}\| = \|\mathcal{Q}_j(T_j - \theta_l s_l) + r_j e_j^T s_l\| = \|r_j e_j^T s_l\| = \|\beta_{j+1} s_j^{(l)}\| = \beta_j^{(l)} \quad (11)$$

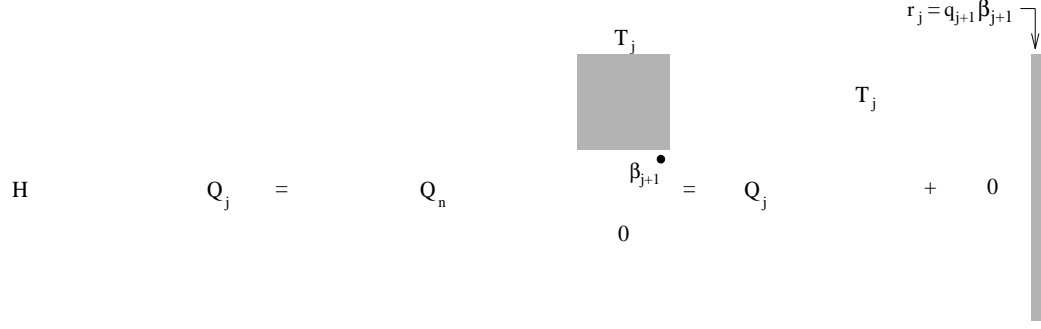


Figure 1: The truncated recurrence.

where  $\|\cdot\|$  denotes the Euclidian norm,  $e_j$  is the last column of the identity matrix of order  $j$ , and  $s_j^{(l)}$  is the bottom element of the eigenvector  $s_l$ . Then, the monitoring of  $\beta_j^{(l)}$  allows the identification of converged solutions, by comparing it with a specified tolerance, and the stopping of the basis generation process. However, a backward error approach gives more reliable results, i.e., an approximate eigenpair should satisfy

$$\frac{\|\mathcal{H}\hat{x} - \hat{\lambda}\hat{x}\|}{\|\mathcal{H}\|} = \frac{\beta_j^{(l)}}{\|\mathcal{H}\|} \leq tol. \quad (12)$$

In fact, in the present implementation,  $\beta_j^{(l)}$  is compared to  $tol \times \|\mathcal{H}\|$ , where  $tol$  is set to the square root of the arithmetic precision and  $\|\mathcal{H}\|$  is specified by the user. If  $\|\mathcal{H}\|$  is set to zero on input, it will be approximated by the largest eigenvalue of  $T_j$  in absolute value.

### 3 The Reduced Problem

In this section, we examine the nature of the matrix  $T_j$  in the reduced problem (10). Equating first the  $j$ -th column of the matrices shown in Figure 1,

$$r_j = \mathcal{H}q_j - q_j\alpha_j - q_{j-1}\beta_j, \quad (13)$$

and multiplying this resulting relation by  $q_j^*$  we get

$$q_j^*r_j = q_j^*\mathcal{H}q_j - q_j^*q_j\alpha_j - q_j^*q_{j-1}\beta_j.$$

However, due to the Gram-Schmidt orthonormalization process ( $q_j^*q_{j-1} = 0$ ) and in order to obtain  $q_j^*r_j = 0$ ,

$$\alpha_j = q_j^*\mathcal{H}q_j.$$

Furthermore,

$$\bar{\alpha}_j = \overline{q_j^*\mathcal{H}q_j} = q_j^T\mathcal{H}^T\bar{q}_j = (q_j^*\mathcal{H}q_j)^T = \alpha_j$$

and thus  $\alpha_j$  is a real number. Then, since  $r_j = q_{j+1}\beta_{j+1}$  and  $q_{j+1}^*q_{j+1} = 1$  for orthonormality conditions,

$$\beta_{j+1}^2 = r_j^*r_j,$$

which is also a real number.

Therefore, the one-vector approach used in our implementation yields a real symmetric tridiagonal matrix as defined in (7). For the solution of the associated reduced eigenproblem a QL method based subroutine, IMTQL, available in EISPACK [7], has been used. Actually, that subroutine has been modified to compute only the bottom entries of each eigenvector of  $T_j s_l = s_l \theta_l$  when the residuals are computed by means of relation (11). The full eigenvectors  $s_l$  are evaluated only for the computation of the approximations  $\hat{x}$ .

On the other hand, in a block strategy the vector  $q_j$  is replaced by a  $n \times p$  matrix  $Q_j$ ,  $r_j$  by a  $n \times p$  matrix  $R_j$ ,  $\alpha_j$  by a  $p \times p$  matrix  $A_j$ , and  $\beta_{j+1}$  by a  $p \times p$  matrix  $B_{j+1}$ . Following the same rules of the above paragraph it follows that

$$A_j = Q_j^* \mathcal{H} Q_j$$

and

$$A_j^* = (Q_j^* \mathcal{H} Q_j)^* = Q_j^* \mathcal{H}^* Q_j = Q_j^* \mathcal{H} Q_j = A_j$$

so that  $A_j$  is Hermitian. Now, in order to obtain  $Q_{j+1}$ , one needs to factor  $R_j$  as

$$R_j = Q_{j+1} B_{j+1}$$

with  $Q_{j+1}^* Q_{j+1} = I$  and  $B_{j+1}$  upper triangular, its diagonal coefficients being real (normalizing factors) and the others generally complex (orthogonalizing factors). Then, the projection of  $\mathcal{H}$  corresponds to the following tridiagonal matrix of dimension  $j \times p$ :

$$T_{j,p} = \begin{bmatrix} A_1 & B_2^* & & & \\ B_2 & A_2 & B_3^* & & \\ & B_3 & A_3 & \ddots & \\ & & \ddots & \ddots & B_j^* \\ & & & B_j & A_j \end{bmatrix}.$$

## 4 The Partial Reorthogonalization

Let us consider the product

$$\eta_{k,j} = \eta_{j,k} = q_k^* q_j \quad (14)$$

which corresponds to the coefficients of the matrix  $Q_j^* Q_j$ . With infinite precision arithmetic

$$\begin{cases} \eta_{k,j} = 1 & \text{for } k = j \\ \eta_{k,j} = 0 & \text{for } k \neq j \end{cases} \quad (15)$$

However, after  $j$  steps in a finite precision arithmetic relations (5) and (15) are not satisfied, so that  $\|I - Q_j^* Q_j\| \neq 0$ , and redundant copies of eigenpairs tend to emerge. This loss of orthogonality is dictated by the introduction of roundoff errors in the operations of Table 1, which can be represented by the introduction of a correction term,  $f_j$ , in equation (13). It is also related with the convergence of a pair  $(\hat{\lambda}, \hat{x})$  and therefore with the eigenvalue distribution of the associated problem [14].

In order to prevent the loss of orthogonality one can apply a full reorthogonalization, instead of using only the two previous vectors computed in the basis generation process. However, such a scheme would strongly increase the number of operations for large values of  $j$  and  $n$ . On the other hand, a preventive measure can be used to keep the orthogonality within a certain level, say  $\|I - Q_j^* Q_j\| \leq \sqrt{\epsilon}$ , for example, where  $\epsilon$  is the arithmetic precision. The basic idea is to monitor the level of orthogonality among  $r_j$  and the vectors of the basis. Then, ignoring for simplicity the roundoff errors introduced in equation (13) and pre-multiplying it by  $q_k^*$  (the  $k$ -th computed vector),

$$q_k^* \mathcal{H} q_j = q_k^* q_{j+1} \beta_{j+1} + q_k^* q_j \alpha_j + q_k^* q_{j-1} \beta_j,$$

and considering the relation (14),

$$q_k^* \mathcal{H} q_j = \eta_{k,j+1} \beta_{j+1} + \eta_{k,j} \alpha_j + \eta_{k,j-1} \beta_j. \quad (16)$$

Rewriting now the equation (13) for the  $k$ -th step and pre-multiplying it by  $q_j^*$ , we get

$$q_j^* \mathcal{H} q_k = q_j^* q_{k+1} \beta_{k+1} + q_j^* q_k \alpha_k + q_j^* q_{k-1} \beta_k,$$

and considering the relation (14) we obtain

$$q_j^* \mathcal{H} q_k = \eta_{j,k+1} \beta_{k+1} + \eta_{j,k} \alpha_k + \eta_{j,k-1} \beta_k. \quad (17)$$

From relations (16) and (17), since  $q_k^* \mathcal{H} q_j = q_j^* \mathcal{H} q_k$  and  $\eta_{k,j} = \eta_{j,k}$ ,

$$\eta_{j+1,k} \beta_{j+1} = \eta_{j,k+1} \beta_{k+1} + (\alpha_k - \alpha_j) \eta_{j,k} + \eta_{j,k-1} \beta_k - \eta_{j-1,k} \beta_j,$$

and taking norms,

$$\eta_{j+1,k} \leq \frac{1}{\beta_{j+1}} [\eta_{j,k+1} \beta_{k+1} + (|\alpha_k| + |\alpha_j|) \eta_{j,k} + \eta_{j,k-1} \beta_k + \eta_{j-1,k} \beta_j], \quad (18)$$

which can be used to estimate the level of orthogonality between  $q_{j+1}$  and  $q_k$ ,  $1 \leq k < j$  (clearly,  $\eta_{j+1,j} \approx \epsilon$ ). All the information required for that is provided by the algorithm at no cost. It should be noted that this strategy was first developed for symmetric matrices [17], with the reorthogonalization being applied only to the vectors with corresponding values of  $\eta$  (the index  $k$ ) above a specified tolerance. However, in the present implementation whenever one  $\eta_{j+1,k}$  becomes larger than  $\sqrt{\epsilon}$ , a full reorthogonalization is applied [13]. Then, all  $\eta$ 's are set to  $\sqrt{n}\epsilon$  and the updating of relation (18) reinitialized. Although it might be seen as a conservative scheme, a stronger level of orthogonality is assured for the subsequent steps of the basis generation process.

## 5 Applications

In this section, we examine 4 different examples in order to illustrate the applicability of the technique described in the previous sections. For the first two examples a small Hermitian matrix has been used: the objective is to show the convergence pattern using  $\mathcal{H}$  and  $\mathcal{H}^{-1}$  (the direct and the inverted operator), since in this case the eigenvalues are



related by their reciprocals (i.e., the inverted spectrum) while the eigenvectors are the same. In the third example the code is used to determine the smallest singular value of a perturbed nonsymmetric matrix (related with an aeroelasticity analysis problem) as a way to evaluate its spectral portrait. Finally, some singular values of a nonsymmetric complex matrix (related with an application in electromagnetism) are computed using an augmented problem strategy. For all cases, the starting vector was generated with random entries, although such a vector can also be specified by the user.

**Application 1.** In this application, we examine the approximate eigenvalues obtained with a basis of size 10 for a Hermitian matrix of dimension 30. The eigenvalue spectrum of the matrix is depicted in Figure 2, so that its Euclidian norm is equal to 60. The approximations are listed in Table 2 in ascending order, as well as the associated residuals defined by relation (11). We can see in that table that mainly the largest eigenvalues begin to convergence, although their residuals are not yet small. On the other hand, there is also some information related with the lower end of the eigenvalue spectrum. The pattern observed is generally typical when a direct operator is employed.

**Application 2.** In this application, we examine the approximate eigenvalues obtained with a basis of size 10 for the inverse of the matrix used in the first application. The reciprocal of the approximations are listed in Table 3 in descending order, as well as the associated residuals. We can see in that table that mainly the small eigenvalues begin to convergence and the residuals are smaller when compared with those of the previous case, although the multiplicity of the first eigenvalue has not yet been detected. On the other hand, it should be noted that in practical applications the matrix does not need to be inverted. If required, one can factor the matrix and then solve systems of equations for  $q_j$ , instead of multiplying by  $\mathcal{H}$ , as indicated in Table 1.

**Application 3.** Many computations involving nonsymmetric matrices may fail in the neighbourhood of singularities. This is basically related with the *nonnormality* of the matrix, which can be expressed by the relation  $\|A^T A - A A^T\| \neq 0$ . One way of studying the “sensitivity” of a matrix consists in the introduction of small perturbations in the entries of the matrix and then examining the resulting perturbed spectrum. The perturbed spectrum can be analysed through the function  $\psi(z) = \log_{10}[\|(A - zI)^{-1}\|_2 \|A\|_2]$ , where  $z$  corresponds to a point in the complex plane and  $\|(A - zI)^{-1}\|_2$  to the largest singular value of  $(A - zI)^{-1}$ . However, it should be noted that this singular value is equivalent to  $1/\sqrt{\lambda_{\min}[(A - zI)^*(A - zI)]}$ , where  $\lambda_{\min}$  indicates the smallest eigenvalue. Therefore, in this application we employ the Hermitian-Lanczos code to determine the spectral portrait  $\psi(z)$  of a nonsymmetric matrix, i.e., to compute the small singular value for different values of  $z$ . The idea is to run the code with the matrix  $(A - zI)^*(A - zI)$  until the smallest eigenvalue of the reduced problem reaches a small residual, which is examined outside the code (some of the largest eigenvalues converge first). The matrix studied has dimension 135. It results from a flutter analysis of an airplane and is labelled “Tolosa” [2, 3, 4]. The spectral portrait obtained is shown in Figure 3, for 3721 values of  $z$  (mesh  $60 \times 60$ ), in the piece of the complex plane defined by the rectangle with vertices  $-50 + 150i$  and  $20 + 200i$ . In that

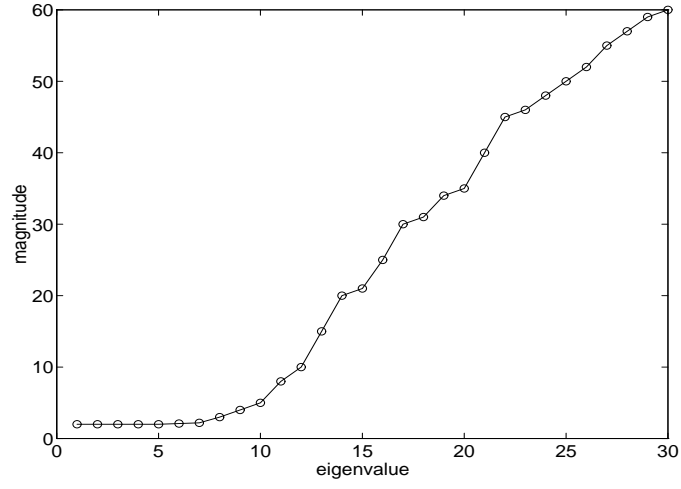


Figure 2: The spectrum of the matrix for Application 1.

Table 2: Eigenvalue approximations for Application 1.

$l$	$\theta_l$	$\beta_i^{(l)}$
1	2.0032	0.5115
2	5.0980	3.7728
3	8.8429	2.9776
4	17.743	5.0323
5	28.342	6.3651
6	32.856	5.7594
7	46.019	5.1082
8	51.083	3.5776
9	56.881	2.3850
10	59.730	1.0282

Table 3: Eigenvalue approximations for Application 2.

$l$	$1/\theta_l$	$\beta_j^{(l)}$
1	53.642	3.5377E-03
2	30.440	8.6636E-03
3	14.940	2.1815E-02
4	8.2144	1.1494E-02
5	5.3617	3.7707E-02
6	4.0245	1.4200E-02
7	3.0032	9.0809E-03
8	2.2017	1.1154E-02
9	2.1017	1.2089E-02
10	2.0000	1.9530E-04

figure, the vertical and horizontal axes give the complex and real parts of the plane, respectively, and the light colours indicate large values of  $\psi(z)$ , whose maximum is 7.23. The norm of the matrix,  $\|A\|_2$ , is equal to  $4.17 \times 10^{+4}$  and 95 steps were required, on average, to reach a residual norm less than  $10^{-8}$  for each smallest eigenvalue, on each point  $z$ . With this application, it is also possible to see the effects of the loss of orthogonality among the vectors. Considering the point  $z = -50 + 150i$ , we have examined the level of orthogonality between  $q_{31}$  (the vector computed at the 31st step) and the previous Lanczos vectors (thus a basis of dimension 31). The Figure 4 shows the norm of the product  $q_k^* q_{31}$ ,  $1 \leq k < 31$ , on a logarithmic scale: the dashed line (with circles) corresponds to the control of the orthogonality level as described in Section 4, and the continuous line (with \*) corresponds to no control. In the first case, 18 eigenvalues have already converged (with residuals less than  $10^{-11}$ ), ranging from 5.2863E+07 to 1.7319E+09 (the largest one for the point  $z$  considered); in the second, spurious copies of the eigenvalues 1.3590E+09, 1.5370E+09 and 1.7319E+09 emerge. Actually, the convergence of solutions begins at the 18th step, which is related with the “plateau” for the first 15 vectors (i.e., the loss of orthogonality). The descent of the solid line in Figure 4 indicates, roughly, that the orthogonality is lost and then “reestablished” after convergence.

**Application 4.** In the study of electromagnetic guided waves the electric and magnetic fields, respectively  $E$  and  $H$ , considering a heterogeneous media and the harmonic case, are given by the Maxwell equations [3, 15]

$$\begin{cases} \text{rot}_\beta E + i\omega H = 0 \\ \text{rot}_\beta H - i\omega E = 0 \\ \text{div}_\beta(\rho E) = 0 \\ \text{div}_\beta(\mu H) = 0 \end{cases}$$

where  $i$  is the complex unit,  $\omega$  the wave frequency,  $\beta$  a propagation constant,  $\mu$  the magnetic permeability and  $\rho$  the dielectric permittivity of the media. Those equations can be discretized by means of a lagrangian finite element formulation. The admissible values of  $\omega$  are then obtained as a function of  $\beta$ , by solving an eigenvalue problem involving a complex non-Hermitian matrix based on  $E$  or alternatively on  $H$ . We consider a matrix of the former type, with dimension 105. Its eigenvalue spectrum is shown in Figure 5 and its singular values are represented in Figure 6. In this application we use the Hermitian-Lanczos code to estimate some singular values of the aforementioned matrix. The strategy employed consists in applying the code to an augmented problem involving

$$\mathcal{H} = \begin{bmatrix} 0 & A \\ A^* & 0 \end{bmatrix}$$

which is complex Hermitian and has eigenvalues appearing as pairs  $(-\lambda, +\lambda)$ , whose modulus lead to the singular values of  $A$  [6]. Then, using a basis of size 60, the Table 4 lists the largest 10 positive eigenvalues. We can see that some of the singular values are already well represented. It is clear that for large values of  $n$  this is probably not the most efficient way to determine all singular values (and vectors). However, such a procedure can be useful in the computation of a few of them, with better numerical properties than the formulation using  $A^*A$ , whose conditioning is squared [8]. In addition, the matrix  $\mathcal{H}$  is not explicitly

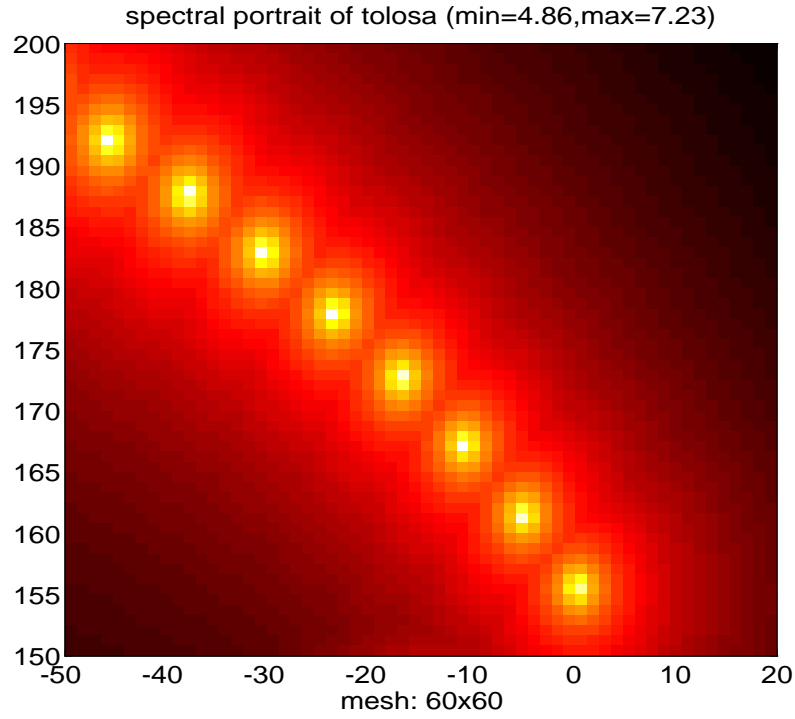


Figure 3: The spectral portrait of Tolosa,  $\psi(z) = \log_{10}[\|(A - zI)^{-1}\|_2 \|A\|_2]$ .

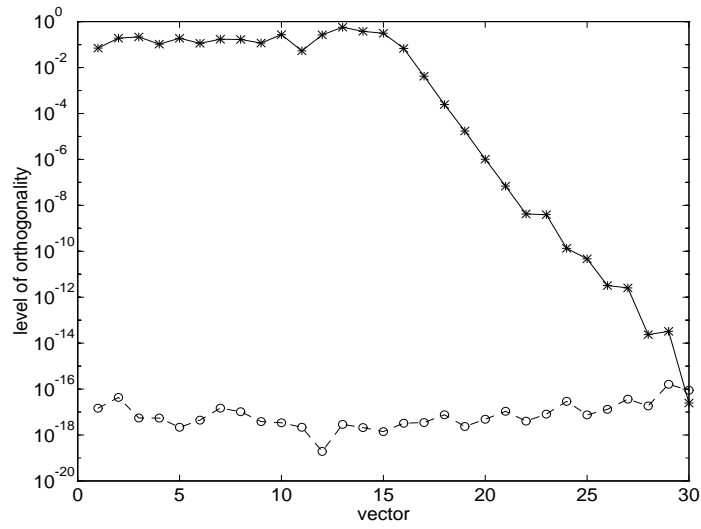


Figure 4: The level or orthogonality,  $q_k^* q_{31}$ ,  $1 \leq k < 31$ .

required, it suffices to keep  $A$ , of dimension  $n$ , and to supply the code with vectors

$$\mathcal{H}q_j = \mathcal{H} \begin{Bmatrix} q_j^{(1)} \\ q_j^{(2)} \end{Bmatrix} = \begin{Bmatrix} Aq_j^{(2)} \\ A^*q_j^{(1)} \end{Bmatrix}$$

for an output vector  $q_j$  of dimension  $2n$ . Therefore, the algorithm generates a basis for a Krylov subspace of the type

$$\mathcal{K}(\begin{bmatrix} 0 & A \\ A^* & 0 \end{bmatrix}, \begin{Bmatrix} q_1^{(1)} \\ q_1^{(2)} \end{Bmatrix}, j) = \text{span}(\begin{Bmatrix} q_1^{(1)} \\ q_1^{(2)} \end{Bmatrix}, \begin{Bmatrix} Aq_1^{(2)} \\ A^*q_1^{(1)} \end{Bmatrix}, \begin{Bmatrix} AA^*q_1^{(1)} \\ A^*Aq_1^{(2)} \end{Bmatrix}, \begin{Bmatrix} AA^*Aq_1^{(2)} \\ A^*AA^*q_1^{(1)} \end{Bmatrix}, \dots).$$

However, as previously suggested by Cullum and Willoughby [6], it is possible to set either  $q_1^{(1)}$  or  $q_1^{(2)}$  to zero. Then, the tridiagonal matrix will have only zero diagonal entries and a save both in numerical operations and storage can be obtained.

## 6 Conclusions

This work described a Lanczos algorithm based code intended for the determination of some eigensolutions of complex Hermitian matrices. One of the main objectives in its implementation was to provide an easy interface for the user. For this purpose, it is given to the user access to intermediate results and to the convergence history, which allows the definition of specific control instructions outside the package. Moreover, the matrix to be analysed is not required internally in the code: until convergence for the solutions required is reached, each time the product  $\mathcal{H}q_j$  has to be computed for a given vector  $q_j$  (or alternatively the solution of a system of equations), the control is returned to the user.

On the other hand, all algebraic operations are carried out by means of BLAS kernels, which helps in achieving portability and a performance enhancement on many computers. Concerning the reorthogonalization strategy, it will ensure a level of orthogonality among the vectors of about the machine precision, as can be seen in Figure 4. Actually, as the basis size increases, more solutions converge and more orthogonalizations are required. However, for some applications, the strategy could possibly be “relaxed” in some way to allow  $\|I - Q_j^*Q_j\| \approx \sqrt{\epsilon}$  and therefore save operations.

In the applications section, the possible utilization of the code was examined by means of distinct study cases, including nonsymmetric real and complex matrices. Concerning the determination of the singular values, we have shown that two different strategies can be applied (a normal equation or an augmented matrix approach, in applications 3 and 4, respectively), depending upon the type of the problem. In this particular, the evaluation of spectral portraits using both of them is currently under investigation and will be subject of following works.

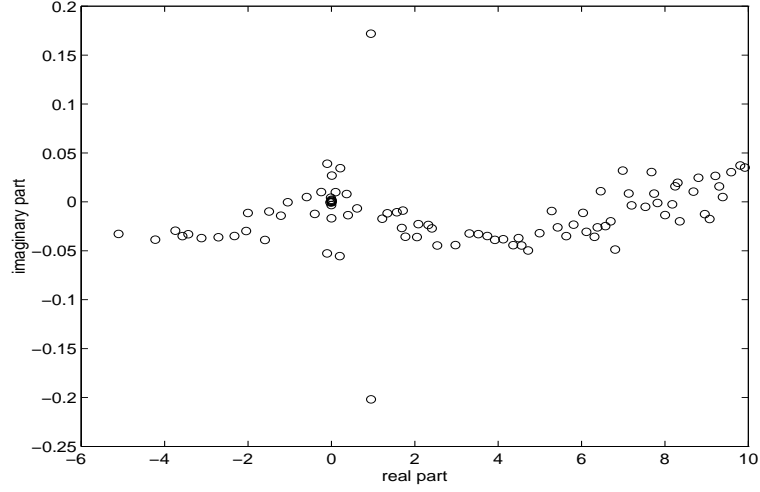


Figure 5: Application 4, spectrum of the matrix ( $n = 105$ ).

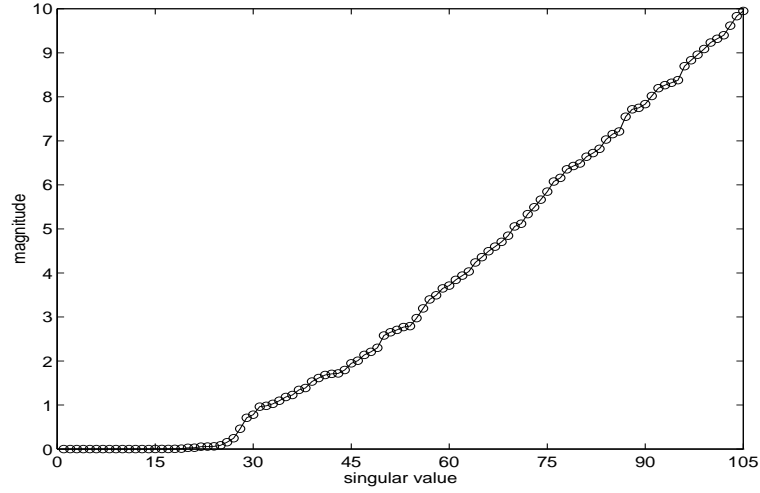


Figure 6: Application 4, singular values of the matrix ( $n = 105$ ).

Table 4: Eigenvalue approximations for Application 4.

$l$	value	residual
1	9.9503	2.4343E-06
2	9.8330	1.7591E-05
3	9.6155	5.9013E-04
4	9.3978	1.7095E-02
5	9.3088	1.2024E-01
6	9.2248	1.0581E-01
7	9.0210	2.2758E-01
8	8.9008	2.4088E-01
9	8.7163	2.1847E-01
10	8.3504	2.5393E-01

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## A User's Guide

The Users' Guide has been moved to a separate file in order to simplify eventual updatings. Please check the directory `doc` in the `hlzpack` distribution. In case of trouble, send an e-mail to `osni@nersc.gov`.